Addition energies of a Quantum Dot with harmonic electron-electron interactions

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We study a two dimensional electron system in a parabolic confining potential and constant magnetic field for the case of harmonic electron-electron interaction. We present analytic results for the electrochemical potential versus magnetic field and discuss the effects of correlation in connection with the addition energy of a Quantum Dot with few electrons.

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Recent achievements of nanolithography in semiconductor technology allow for the fabrication of devices in which a definite number of electrons are confined within two-dimensional islands of size as small as tenths of nanometers [Quantum Dots (QD)] [1]. In the last few years there has been growing interest in the study of these devices in view of improving our understanding of correlated electron systems. In fact, QD are unique with respect to other structures, e.g., macromolecules and clusters, because a dot can be connected to sources and/or a measuring apparatus via contacts. This possibility allows investigation of the system with probes changing the number of particles [2]. Indeed, quite recently Tarucha *et al.* [3] have measured the tunneling current in gated vertical quantum dots as a function of a magnetic field B applied parallel to the current. In the Coulomb blockade regime and in presence of a very small voltage bias, the current shows a sequence of peaks that occur whenever the gate voltage V_g is proportional (via a voltage-to-energy conversion coefficient) to the chemical potential $\mu_N = E(N) - E(N-1)$ for adding one more particle to the dot. Here $E(N)$ is the ground-state (GS) energy of the dot once N electrons are localized in it.

General features of the current peaks are qualitatively reproduced by assuming that electrons are confined by a parabolic potential of frequency ω_0 and by adding the charging energy $E_{\rm ch} = V_0 N(N-1)/2$ to account for the electron-electron repulsion [Constant Interaction (CI) model] [3,4]. The GS energy is obtained, for any value of B, by filling the lowest one-particle free harmonic oscillator levels with electrons of both spin. In this model the observed increasing of the addition energy $\Delta_N = E(N+1) + E(N-1) - 2E(N)$ for $N = N_p$, where $N_p = 2, 6, 10, 20, ...$, is easily related to the shell structure of the two dimensional harmonic potential spectrum, which leads to a marked increase of μ_N whenever a new shell is opened. The CI model then reproduces the oscillations of the current peaks with the field B as well as their shift in pairs. Because the CI GS wave function has minimum total spin, its agreement with the experimental pattern also confirms that in some QD, like the one in Ref. [3], the effective g-factor g_* can be very small [5]. However, there are some evident features of the experiments that cannot be reproduced by the simple independent electron CI Hamiltonian. Because the harmonic single-particle levels are equally spaced, according to the CI model (at $B = 0$) Δ_N should be constant ($\Delta_N = V_0$) within a unfilled shell. For the same reason one should then find $\Delta_{N_p} = V_0 + \hbar\omega_0$ for any N_p. While the experimental pattern in Ref. [3] allows a clear identification of a shell structure for dots of less than ≈ 20 electrons, it also clearly shows a smooth shrinkage of the spacing Δ_N within a unfilled shell with growing N, as it was previously noticed in single electron capacitance spectroscopy [6]. Then, one observes that the expected peaks at Δ_{N_p} decrease in height each time a new shell opens. In general, as discussed by Schmidt *et al.* [7], fittings of capacitance data within the CI model indicate that the confinement strength of the potential appears to decrease rapidly with increasing energy. Question arises whether such an effect can be attributed to electron-electron correlation.

In this letter we consider the model of harmonic interactions (HI) between N electrons [8] in a parabolic confining potential. Although there is tenuous justification for this model interaction, when the magnetic field is not too small and the electron number not too large we show that it embodies correlation effects which correctly reproduce interesting experimental features. The model is well known and its popularity relies on the fact that for fully spin polarized electrons the Laughlin trial wave function, which is successful in describing the Coulomb gas in a quantizing magnetic field, has a form similar to one of its eigenstates [9]. Successively, the model has been discussed, again in the fully polarized spin sector, in connection with the QD problem in a large magnetic field orthogonal to the dot plane [10]. In view of the finding $g_* \approx 0$, results about the maximum spin sector are not relevant to the present discussion. We present some details of the solution because little information can be found in literature about the GS wave function in an arbitrary spin sector.

We do not expect the HI model useful in discussing the region of small magnetic field. In fact, there are evidences [3] that in this case the spin sector of the QD GS obeys Hund's rule, whereas the GS of the HI model at $B = 0$ has necessarily lowest spin [11]. Instead, for higher magnetic field our results closely reproduce features of

the experimental data of Ref. [3] and are summarized in Fig. (1). The narrowing, compared with the CI model, of the distance between current peaks is transparent. The shift, at fixed V_0, of the orbital angular momentum transitions which take place with increasing B to lower values of the magnetic field also clearly appears in our results. Then, close to the point where the oscillations in the peak location drop, for large enough N, the peaks making up a pair have an intriguing "out of phase" behaviour, similar to the experimental pattern.

The HI Hamiltonian in a constant magnetic field B is $H_B = H_0 + \hbar\omega_c(L_3 + g_* S_3)/2$, where $\hbar L_3 = \sum_{i=1}^N (x_{1,i}p_{2,i} - x_{2,i}p_{1,i})$ and $S_3 = \sum_{i=1}^N S_{3,i}$ are the third component of the total angular momentum and total spin operators, respectively, $\boldsymbol{r}_i = (x_{1,i}, x_{2,i})$ and $\boldsymbol{p}_i = -i\hbar\partial/\partial\boldsymbol{r}_i$ are the coordinates and momentum of the i-th electron, $\omega_c = eB/(m_* c)$ is the cyclotron frequency, and

$$H_0 = -\frac{\hbar^2}{2m_*}\sum_{i=1}^N \frac{\partial}{\partial \boldsymbol{r}_i}\cdot\frac{\partial}{\partial \boldsymbol{r}_i} + m_*\frac{\omega^2}{2}\sum_{i=1}^N |\boldsymbol{r}_i|^2 + \sum_{1\le i<j\le N}(V_0 - \frac{U}{2}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2). \qquad (1)$$

Here m_*, g_* denote effective parameters and for the time being we set $m_* = e = \hbar = 1$. The frequency $\omega^2 = \omega_0^2 + \omega_c^2/4$ enters H_0 upon choosing the gauge $\boldsymbol{A} = (B/2)(-x_2, x_1)$ for the vector potential and represents the frequency of the effective parabolic confining potential, whereas $U \ge 0$ is the strength of the interaction. For $U = 0$ then H_B reduces to the CI model. Introducing $\Lambda_{ij} = \Omega^2\delta_{ij} + U\mathcal{J}_{ij}$, where $\Omega^2 = \omega^2 - NU$ and $\mathcal{J}_{ij}$ denotes the matrix with all unit entries, (i.e., $\mathcal{J}_{ij} = 1\ \forall\, i,j$), the potential energy entering Eq. (1) can be compactly written as $V = \sum_{i,j=1}^N \Lambda_{ij}\boldsymbol{r}_i\cdot\boldsymbol{r}_j/2$, so that H_0 is bound from below if Λ_{ij} is positive definite. The symmetric matrix Λ_{ij} is diagonalized by any unitary matrix $\mathcal{U}_{i\nu}$ satisfying to $\sum_{i=1}^N \mathcal{U}_{i\nu} = 0$, $\forall\nu \ne N$, and $\mathcal{U}_{iN} = N^{-\frac{1}{2}}$, $\forall i$. Its eigenvalues $\lambda_1 = \ldots = \lambda_{N-1} = \Omega^2$, $\lambda_N = \omega^2$ are readily evaluated, so that positivity is ensured whenever $\omega^2 > NU$. Hence, if we limit the discussion to N not too large, the unphysical feature of dealing with an interaction unbounded at large distances is compensated by the presence of the confining potential. We then introduce normal coordinates $\boldsymbol{y}_\nu = \sum_{i=1}^N \mathcal{U}^\dagger_{\nu i}\boldsymbol{r}_i$. The Laplacian $\Delta = \sum_{i=1}^N \partial/\partial\boldsymbol{r}_i\cdot\partial/\partial\boldsymbol{r}_i$, the angular momentum L_3, and the operator $R^2 = \sum_{i=1}^N |\boldsymbol{r}_i|^2$ are invariant under unitary transformations and from the invariance of R^2 one gets the simple but key identity $\sum_{\nu=1}^{N-1}|\boldsymbol{y}_\nu|^2 = \sum_{i<j}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2/N$. In the new basis the equation $H_B\Psi = E\Psi$ is immediately solved, because the key identity allows to write H_0 as a sum of separated harmonic oscillators of frequencies $\sqrt{\lambda_\nu}$. However, the straightforward normal-mode approach is of no much practical help, because the main problem one faces is to account for the identity of the particles. Eigenfunctions of H_B with definite symmetry under particle permutations can be factorized in the form $\Psi = \Psi_{\rm cm}\Psi_r$, in the usual way [12], where $\Psi_{\rm cm}$ is the completely symmetric harmonic wave function of the center of mass (c.m.) coordinate $\boldsymbol{r} = N^{-\frac{1}{2}}\boldsymbol{y}_N$, with energy $E_{\rm cm}$ and angular momentum $L_3^{\rm cm}$, while the relative motion wave function Ψ_r must be solution of the equation

$$-\frac{1}{2}\Delta\Psi_r + \frac{\Omega^2}{2N}\sum_{i<j}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2\Psi_r + \frac{\omega_c}{2}(L_3 + g_* S_3)\Psi_r = (E - E_{\rm ch} - E_{\rm cm} - \frac{\omega_c}{2}L_3^{\rm cm})\Psi_r, \qquad (2)$$

of same symmetry as Ψ and of zero total linear momentum $\boldsymbol{P} = \sum_{i=1}^N \boldsymbol{p}_i$.

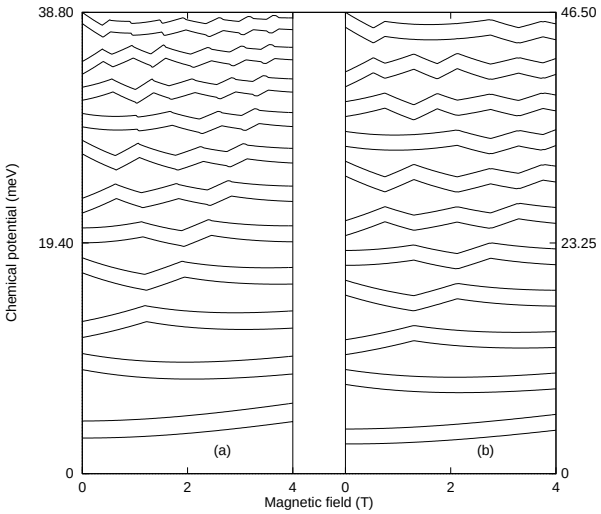

FIG. 1 Chemical potential μ_N versus magnetic field B for $N \le 22$: (a) HI model for $\hbar U/(m_*\omega_0) = 0.07$ meV; (b) CI model. Parameter values are $\hbar\omega_0 = 3$ meV, $\hbar\omega_c/B = 1.63$ meV/T, $V_0 = 1.5$ meV, $g_* = -0.03$.

Henceforth we need only consider the lowest energy c.m. wave function and for the time being we thus set $\Psi_{\rm cm} = \exp\{-\omega\sum_{i,j=1}^N \boldsymbol{r}_i\cdot\boldsymbol{r}_j/(2N)\}$, for which one has $E_{\rm cm} = \omega$ and $L_3^{\rm cm} = 0$. If one looks for eigenstates of Eq. (2) in the form $\Psi_r = \Phi\Psi_0$, where $\Psi_0 = \exp\{-\Omega\sum_{i<j}|\boldsymbol{r}_i - \boldsymbol{r}_j|^2/(2N)\}$, and employes holomorphic coordinates $z_i = x_{1,i} + ix_{2,i}$, and $\bar{z}_i = x_{1,i} - ix_{2,i}$, one gets that the unknown function Φ must satisfy the couple of equations

$$-\sum_{i=1}^N(2\bar{\partial}_i\partial_i - \Omega_+ z_i\partial_i - \Omega_-\bar{z}_i\bar{\partial}_i)\Phi + \frac{\omega_c}{2}g_* S_3\Phi = (E - \mathcal{E}_0 - E_{\rm ch})\Phi, \qquad \boldsymbol{P}\Phi = 0, \qquad (3a,b)$$

where $\mathcal{E}_0 = \Omega(N-1) + \omega$ is the zero-point energy, $\Omega_\pm = \Omega \pm \omega_c/2$, and we have used the shorthand notation

$\partial_i = \partial/\partial z_i$, and $\bar\partial_i = \partial/\partial \bar z_i$. Because the function Ψ_0 is completely symmetric, Ψ_r and Φ must have same symmetry. Eq. (3a) is a sum of N separated Hamiltonians and its solutions are built up in terms of single-particle orbital wave functions f_{n_1,n_2}, with eigenvalues ε_{n_1,n_2},

$$f_{n_1,n_2} = e^{\Omega \bar z z} \bar\partial^{n_1} \partial^{n_2} e^{-\Omega \bar z z},$$
$$\varepsilon_{n_1,n_2} = \Omega(n_1+n_2) + \frac{\omega_c}{2}(n_1-n_2), \qquad (4)$$

where n_1 and n_2 are non negative integers. Apparently, the original interacting problem reduces to a free problem and the main effect of the interaction seems just related to a redefinition of the effective frequency $\omega \to \Omega$. However, Eq. (3b) is highly non trivial and already the two-particle problem shows that it can be satisfied in general only by taking linear combinations of degenerate N-particle solutions. Moreover, the frequency $\Omega = \sqrt{\omega^2 - NU}$ depends on N, so that energy differences like $E(N) - E(N-1)$ cannot be analyzed in terms of one-particle levels. In these respects the system is correlated.

Fortunately, as expected on general ground, one can easily check that the ordinary Slater determinant Z obtained by filling the N lowest states (4) (so that $S_3 = N/2$) is a solution of *both* Eqs. (3a,b). Fig. (2) shows some typical shape of the set of occupied levels. By increasing B one observes a depletion of the levels in the SE side and an extra filling in the NW side, because the contribution $H_L = \omega_c L_z/2$ favours decrease of the orbital angular momentum. Noticing that the functions f_{n_1,n_2} are polynomials and using standard properties of determinants under column addition and multiplication, it is easy to see that for any set of the form depicted in Fig. (2) the Slater determinant can be rearranged into the compact form $Z = \det[z_i^{n_1} \bar z_i^{n_2}]$. This expression is invariant under translation $z_i \to z_i + z_0$, $\forall i$, so that $\boldsymbol{P} Z = 0$ as requested. Introducing the spin index $\sigma = 1, 2$ for up and down electrons, respectively, it follows that the GS wave function $\Psi_{\rm GS}$ of H_B in the spin sector $S_3 = (M_1 - M_2)/2$, $N = M_1 + M_2$, is obtained, up to a normalization constant, by antisymmetrizing the product of the spin-up and spin-down wave functions. Denoting $\mathcal{A}$ the antisymmetrization, we formally have

$$\Psi_{\rm GS} = \exp\{-\frac{1}{2}\sum_{i,j=1}^{N} \bar z_i \Gamma_{ij} z_j\} \times \mathcal{A}\left\{ \prod_{\sigma=1}^{2} \det[z_{i_\sigma}^{n_1^\sigma} \bar z_{i_\sigma}^{n_2^\sigma}] \chi_\sigma \right\}, \qquad (5)$$

where z_{i_σ}, with $i_1 = 1, \ldots, M_1$ and $i_2 = M_1 + 1, \ldots, N$, are the coordinates of spin-up and spin-down electrons, respectively, χ_1, χ_2, are the totally symmetric spin functions of spin-up and spin-down electrons, and (n_1^σ, n_2^σ) are the labels of the (lowest energy) levels occupied by spin-σ electrons. The matrix $\Gamma_{ij} = \Omega\delta_{ij} + N^{-1}(\omega - \Omega)\mathcal{J}_{ij}$ is the square root of Λ_{ij} and enters Eq. (5) upon combination of Ψ_0 with the c.m. GS wave function.

For zero magnetic field the GS is obtained by filling consecutively the levels along successive diagonals $n_1 + n_2 = k$, $k = 0, 1, ...$ with two electrons of opposite spin, so that $\Psi_{\rm GS}$ has $S_z = 0$ or $S_z = \pm 1/2$. Completion of a diagonal corresponds to one more shell filled. When the magnetic field is turned on, for a wide range of B the GS remains in the lowest spin sector due to the smallness of g_*, whereas as previously seen the shape of the Fermi sea modifies in order to lower the orbital angular momentum.

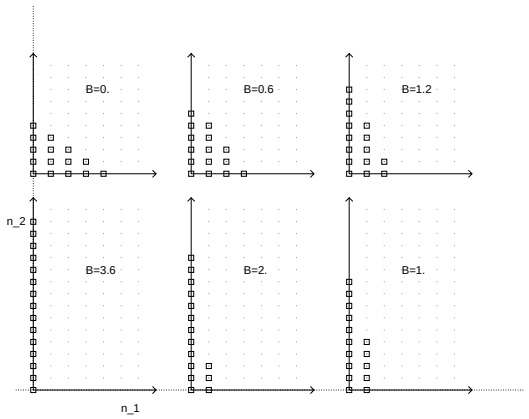

FIG. 2 Occupied single-particle quantum numbers (n_1, n_2) of 15 spinless fermions for six different values of the magnetic field B (T). Parameter values are the same as in Fig. (1a).

The lowest attainable value of the orbital angular momentum $L_3^{\rm min} = -\sum_\sigma M_\sigma(M_\sigma - 1)/2$ is obtained by filling the levels $(n_1^\sigma, n_2^\sigma) = (0, m_\sigma)$, where $m_\sigma = 0, 1, \ldots, M_\sigma - 1$. In this case the Vandermonde determinant $Z = \det[\bar z_i^m] = \prod_{i<j}(\bar z_j - \bar z_i)$ allows a closed expression for the GS wave function $\Psi_{\rm GS}^L$. Denoting $\{\boldsymbol{r}_i, \sigma_i\}$ orbital and spin coordinates of the i-th electron, Eq. (5) gives the Laughlin-like [13] state

$$\Psi_{\rm GS}^L = \exp\{-\frac{1}{2}\sum_{i,j=1}^{N} \bar z_i \Gamma_{ij} z_j\} \times \prod_{i<j} (\bar z_j - \bar z_i)^{\delta_{\sigma_i,\sigma_j}} e^{i\frac{\pi}{2}{\rm sign}(\sigma_i - \sigma_j)}. \qquad (6)$$

Our results for the chemical potential vs. magnetic field are shown in Fig. (1). The curves are splitted by the charging energy V_0 but the N-dependence of Ω leads to a sizeable reduction of the energy scale of the HI model compared with the CI model. This behaviour is in agreement with the experimental pattern of Ref. [3] and with the discussion in Ref. [7]. Although one cannot overestimate the model nature of the harmonic interaction, our results indicate that the rapid decrease of the confinement strength with increasing electron num-

ber can be due to pure correlation effects. The curves (for $N \geq 5$) perform oscillations that signal transitions to states of lower L_3, and drop at the field value where the minimum angular momentum state (6) becomes energetically favourable. It is easy to see that this happens when $2\Omega/\omega_c \leq M_1/(M_1-2)$ (with $M_1 \geq M_2$). In the CI model the curves are perfectly paired because of the spin degeneracy of the one-particle levels. For example, the transition to the state of lowest L_3 takes place when $2\omega/\omega_c = M_1/(M_1-2)$. This relation gives the same value of the magnetic field at which the transition takes place both for $N = 2M$ and for $N = 2M-1$. Instead, in the HI model the N-dependence of Ω breaks this perfect pairing, in particular for large N where Ω becomes small. While usually the angular momentum of the GS is a decreasing function of the number of particles, at the field values where the paired curves come out of phase one instead finds $L_z(2N-1) \leq L_z(2N)$. For instance, at $B = 3.6$ T one has $L_z(21) = -89$, whereas $L_z(22) = -88$. Hence, the strong reduction of the escillator frequency at large N allows for level crossing even within a single pair of particles which are added with opposite spin. This in turn leads to the oscillations out of phase of the peaks forming a pair, a feature which is absent in the CI model. We conclude that, in spite of the simplicity of the model for including electron-electron correlations, many features of the experiment of Ref. [3] are nicely reproduced.

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